TACC IN 2020: COVID-19, AND THE NEXT GENERATION OF CYBERINFRASTRUCTURE

TACCSTER MEETING

Dan Stanzione
Executive Director
Associate Vice President for Research

September 2020

WELCOME AND THANK YOU!

2020 HAS BEEN A CHAOTIC BUT IMPACTFUL YEAR FOR TACC

- First year of Frontera Operations!
- First Year of Planning for the Leadership Computing Facility
- Renewals of many of our largest projects
- Continued push in new technologies
- An industry not sure where to go in architecture
- More and more AI
- And, of course, COVID-19.

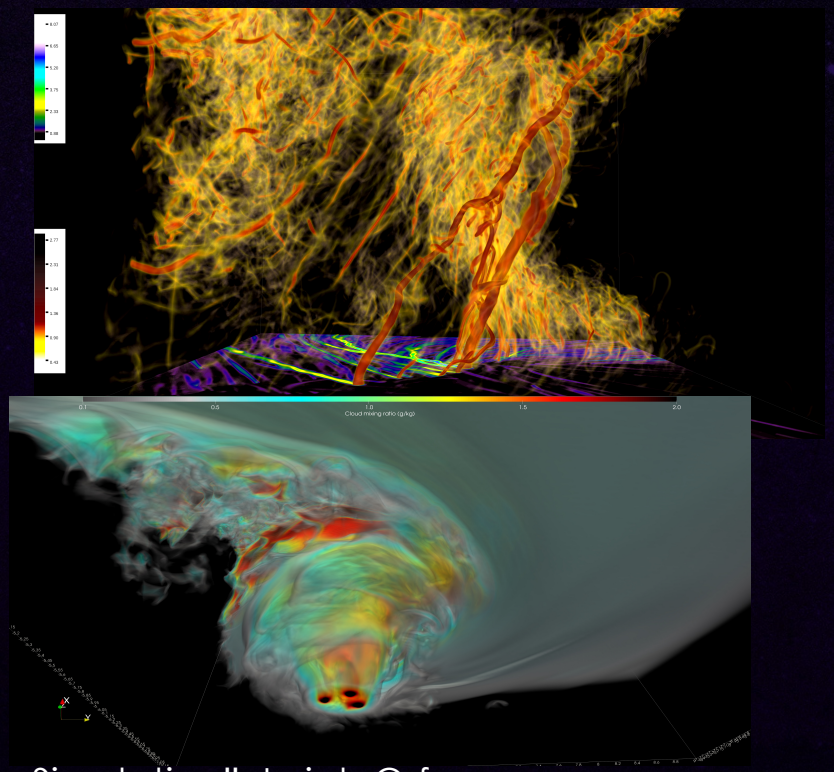
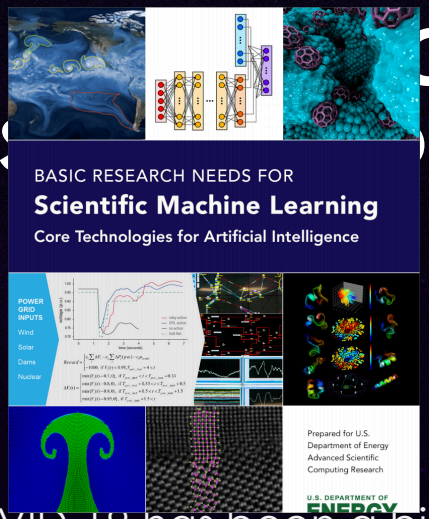


Figure: "World's Most Detailed Tornado Simulation", Leigh Orf, Wisconsin – used more than 200,000 cores on Frontera

FRONTERA VIRTUAL TOUR

THE *COMPUTATIONAL* SCIENCE AT SCALE NO S F NEEDS. . . NOW MORE THAN EVER.



Review | Open Access | Published: 07 February 2020

Eleven grand challenges in single-cell data science

David Lähnemann, Johannes Köster, [...] Alexander Schönhuth

Genome Biology **21**, Article number: 31 (2020) | Cite this article

Mapping the human brain: comparing the US and EU Grand Challenges†

Dolores Modic, Maryann P. Feldman Author Notes

Science and Public Policy, Volume 44, Issue 3, June 2017, Pages 440–449, https://doi.org/10.1093/scipol/scw085

AMS Grand Challenges in Big Data and Earth Sciences

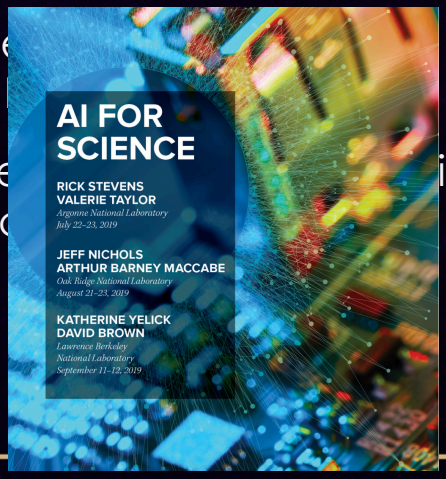
EDITOR'S CHOICE

Grand Challenges in Comparative Physiology: Integration Across Disciplines and Across Levels of Biological Organization

Donald L. Mykles, Cameron K. Ghalambor, Jonathon H. Stillman, Lars Tomanek

Integrative and Comparative Biology, Volume 50, Issue 1, July 2010, Pages 6–16, https://doi.org/10.1093/icb/icq015

Published: 21 April 2010



- COVID-19 has been a big pa tl
- "Urge pa e one
- There ide oss industry, of ind at- AI.

Procedia Computer Science
Volume 108, 2017, Pages 1811-1812

ELSEVIER

Multiscale Modelling and Simulation, 14th International Workshop

Derek Groen, Bartosz Bosak, Valeria Krzhizhanovskaya, Alfons Hoekstra, Petros Koumoutsakos

Physics > Atmospheric and Oceanic Physics

[Submitted on 21 Nov 2019]

Confronting Grand Challenges in Environmental Fluid Dynamics

T. Dauxois, T. Peacock, P. Bauer, C.P. Caulfield, C. Cenedese, C. Gorlé, G. Haller, G.N. Ivey, P.F. Linden, E. Meiburg, N. Pinardi, A.A. Sepp Neves, N.M. Vriend, A. Woods

Environmental fluid dynamics underlies a wealth of natural, industrial and, by extension, societal challenges. In the coming decades, as we strive towards a more sustainable planet, there are a wide range of grand challenge problems that need to be tackled, ranging from fundamental advances in understanding and modeling of stratified turbulence and consequent mixing, to applied studies of pollution transport in the ocean, atmosphere and urban environments. A workshop was organized in the Les Houches School of Physics in France in January 2019 with the objective of gathering leading figures in the field to produce a road map for the scientific community. Five subject areas were addressed: multiphase flow, stratified flow, ocean transport, atmospheric and urban transport, and weather and climate prediction. This article summarizes the discussions and outcomes of the meeting, with the intent of providing a resource for the community going forward.

COMPUTATIONAL SCIENCE IN AN ERA OF TRANSITION

- Computational science and engineering is in a period of transition:
  - Toward more complex models: multiphysics, multiscale, multirate, multimodel **(10x-100x scale up)**
  - From forward simulation to "outer loop" problems: uncertainty quantification, inverse problems, data assimilation, optimal design, optimal control, simulation-based decision-making (all involve principled exploration of parameter space) **(100x-1000x scale up)**
  - Increasing role of data-driven and data-intensive computing
  - Increasing role of statistical models and machine learning **(possible 10x-100x scale down… or up).**
- Computer architectures and programming models are also in the midst of a transition toward significantly increased complexity, heterogeneity, concurrency
- Critical that the three A's—**architectures, algorithms, and applications**—evolve in an integrated and coordinated way

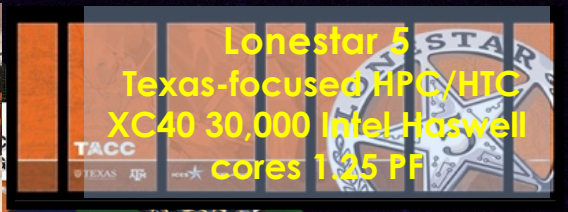
THE WHOLE ECOSYSTEM IS NEEDED FOR DISCOVERY

- Very few of our problems are "just simulation" or "just AI".
- The modes of computation are varied (more interactive, more near real-time, more long term mission needs).
- The hardware itself is overwhelmingly complex:
  - *"Less talked about is how the shift to massive parallelism and heterogeneity has broken how performance scales in both performance and cost".*
- Add in all the parts of discovery, from instrument to computation to analysis, and the complexity is no longer something "a brilliant grad student" can manage alone.

ECOSYSTEM IS THE RIGHT WORD

FRONTERA

Leadership/Discovery Science



- V
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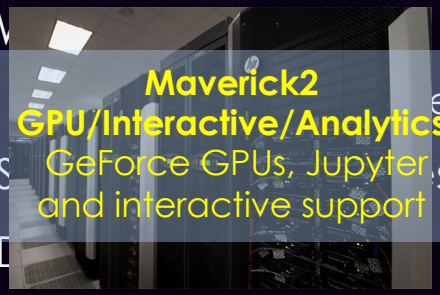
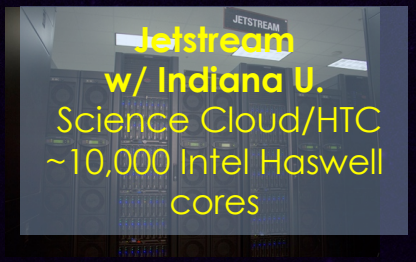
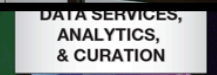
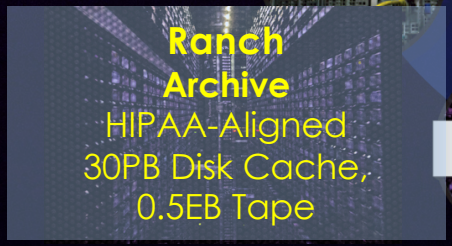
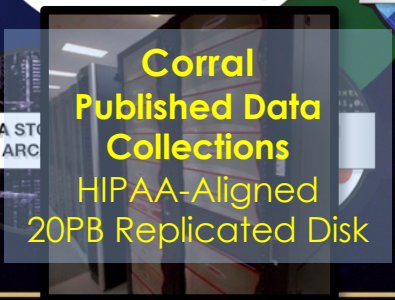
- People who can use it.











9/18/20

TACC IS HERE TO HELP!

- Computation
  - HPC
  - Interactive
  - As-a-Service
- Data
  - Storage
  - Management/Curation
  - Visualization
- People and Consulting
  - Support
  - Performance tuning
  - Web/Portals
  - Workflow
  - Parallelization
  - Proposal Support!
- Training

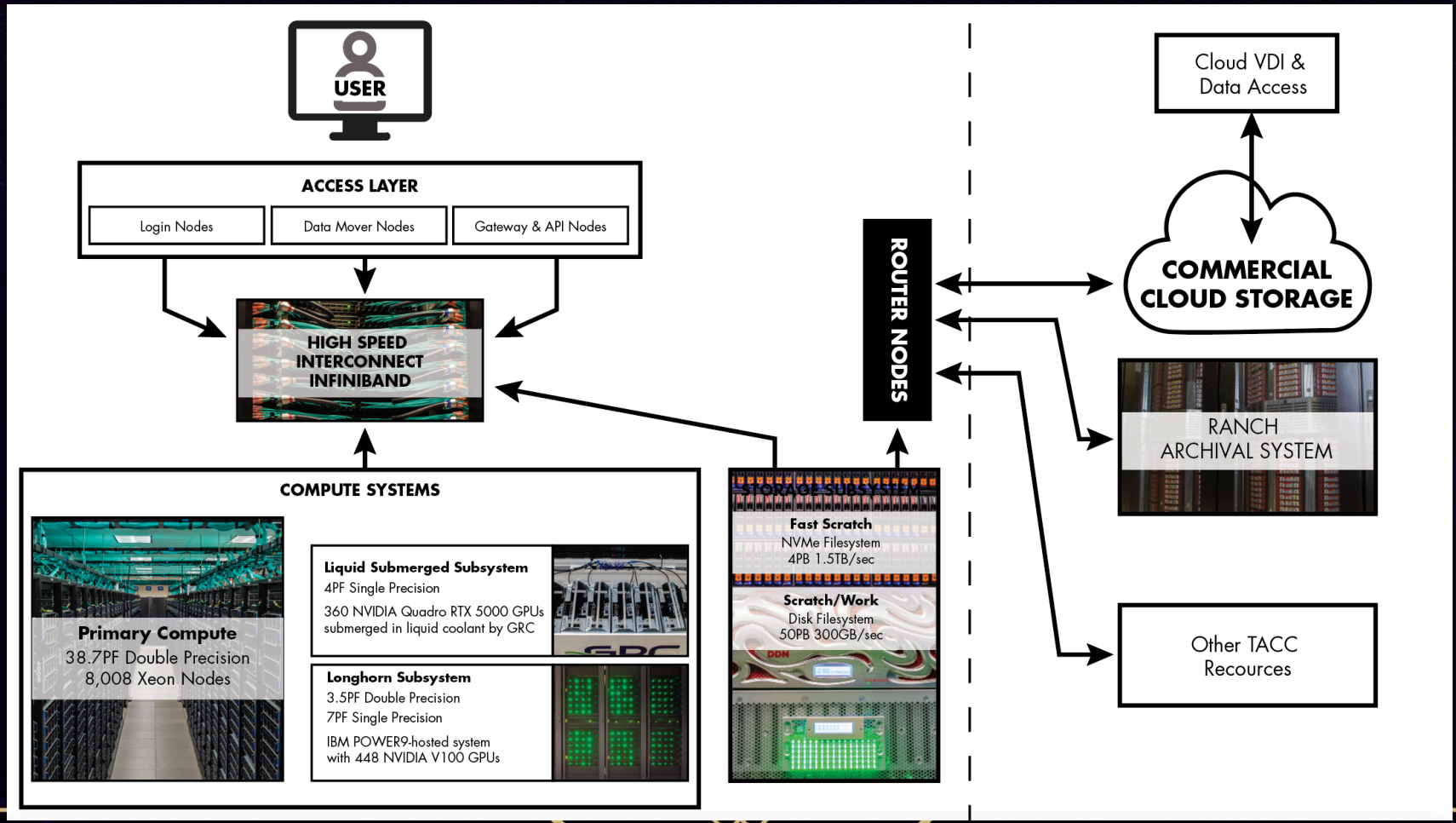
YEAR 1

- About 30% of the time has been diverted to emergency COVID response work since March.
- Number of Jobs run: **Over 1 Million (1,091,118)**
- Node hours delivered: **50M (2.5 Billion+ Core Hours)**
- Uptime is over 96%; the CPU and 2 GPU systems all have utilizations of 80% or higher.
- Cybersecurity incidents: **ZERO**

YEAR 1

- Top 500, still #8. I/O 500, #3
- Portal is up and running
- Commercial cloud integration is functional with Azure, AWS
- Founding partner in the COVID-19 HPC Consortium
- First class of Fellowships underway.

FRONTERA IS A GREAT MACHINE – AND MORE THAN A MACHINE



FRONTERA – RTX SUBSYSTEM

- 90 nodes
- 4 NVIDIA Quadro 5000 RTX cards per node
- 16 GB per card
- 11 TFlop single-precision per card
- Mineral oil-cooled immersion
- Additional GPU modules
- Accessed via rtx queues

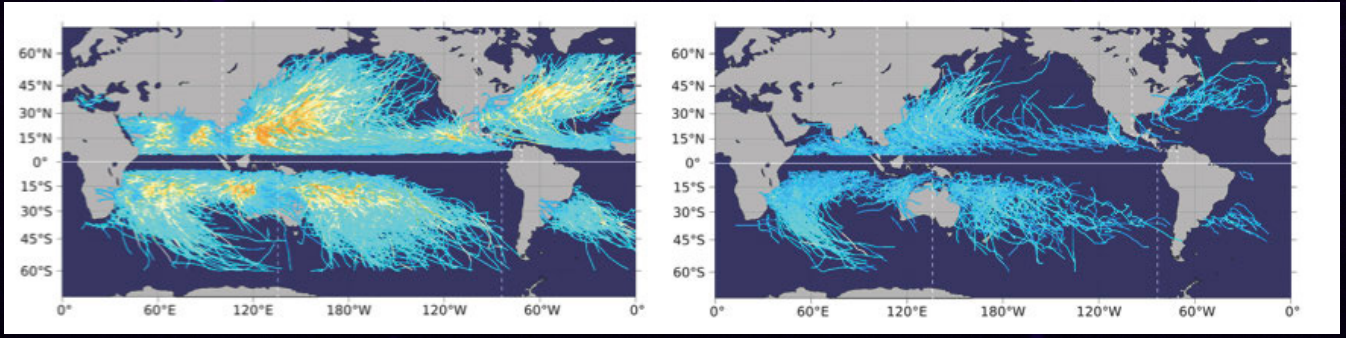
LONGHORN

If you have used DOE's *Sierra* system at Livermore, it's that.

- 104 IBM Power9 nodes
- 4 NVIDIA V100 GPUs per node
- V100s connected with NVLINK on node
- 7 TFlop double-precision performance per card
- 14 TFlop single-precision performance per card
- 16 GB per card

FRONTERA BRIDGES TO THE COMMERCIAL CLOUD:
NEW HIGH-RESOLUTION GLOBAL CLIMATE MODEL PREDICTS CHANGES TO EXTREME WEATHER, OCEAN CURRENTS

- Ping Chang, Texas A&M (collaborators at NCAR and QNLM).
- CESM, 25KM resolution
- One of the UN-supported HighResMIP simulations – the official climate change forecasts.
- In addition to large simulations, also published the data results to Azure, where they do online analytics on ~550GB of data with the "PanGeo" Cloud platform.

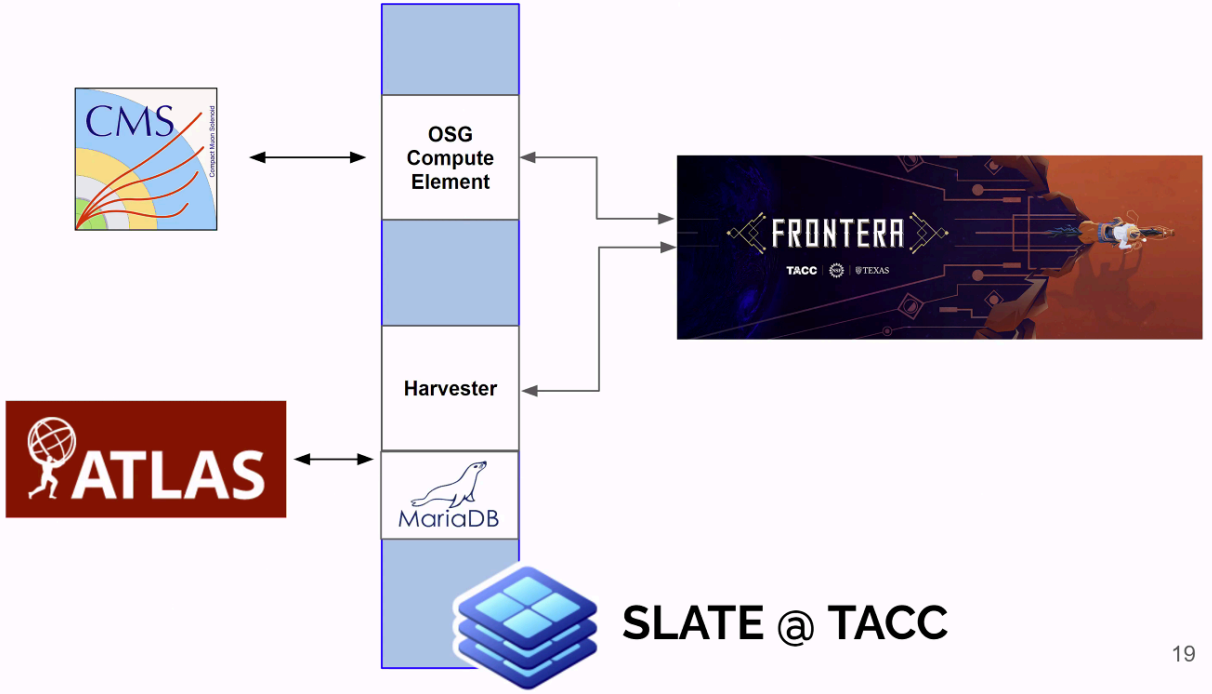


FRONTERA AS-A-SERVICE: EMBEDDING IN AUTOMATED WORKFLOWS: *WORKFLOW SUPPORT IN HIGH ENERGY PHYSICS*

Examples of Federated Operations

Gateways

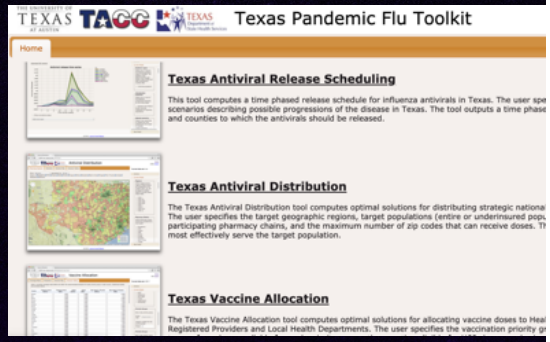
U.S. ATLAS and U.S. CMS are both investigating or developing SLATE-based solutions for sending workloads to the Frontera supercomputer at TACC.

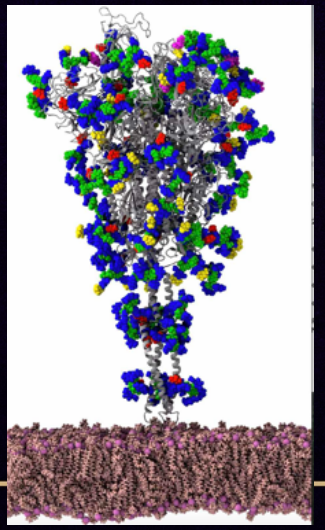


19

CORONAVIRUS RESPONSE
COMPUTATIONAL APPROACHES TO ATTACK AN EPIDEMIC

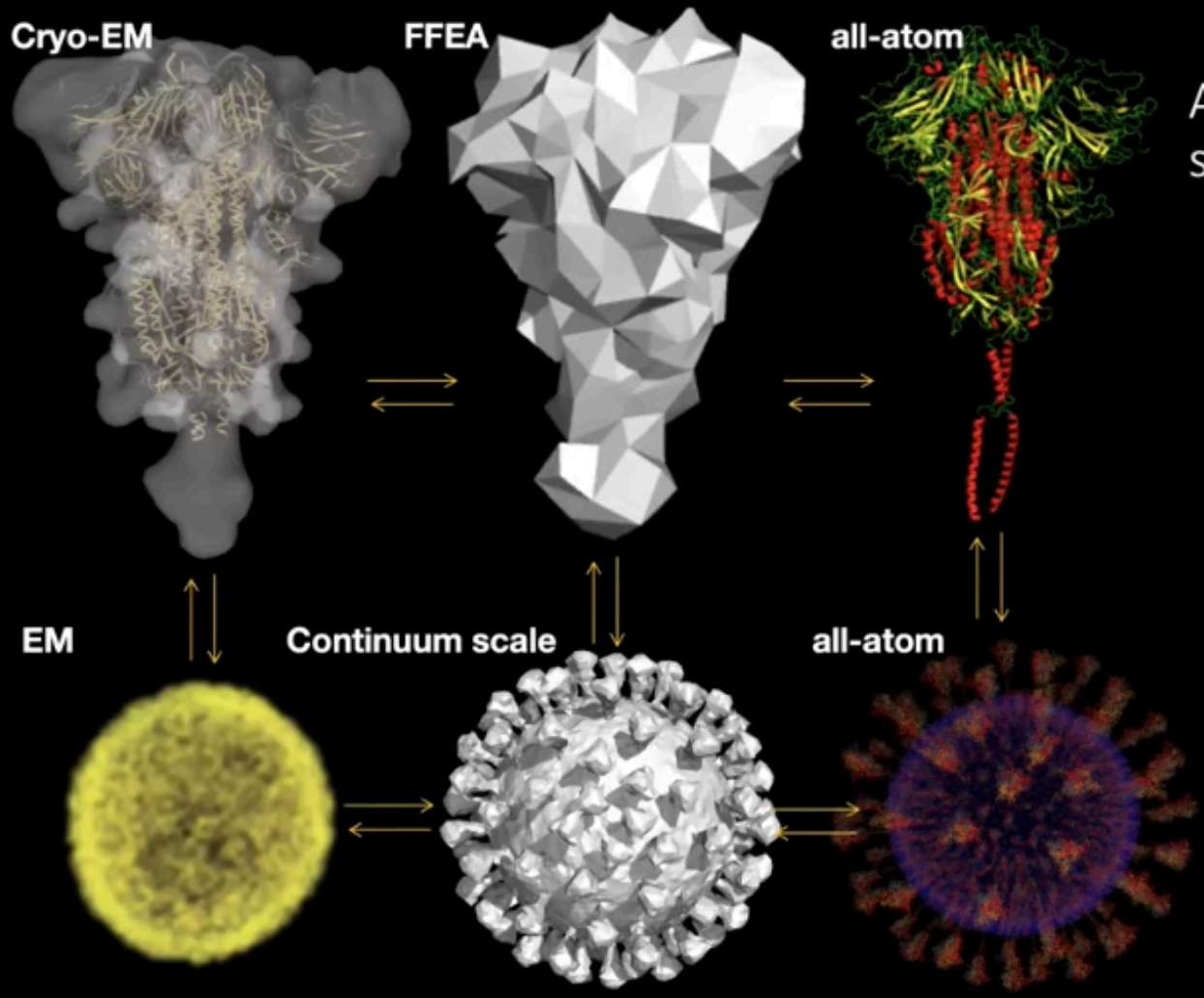
- **People and Resources**
  - **Computational Epidemiology** – aims to model the spread of the virus and the impact a pandemic could have on critical social services (police, fire, healthcare, etc.) in communities, regions and countries.
- **Proteins and Molecules**
  - **Whole Viron Structural Modeling -** Atomic scale molecular dynamics to understand the structure of the virus
  - **Computational drug screening** – Docking and Folding - Aims to accelerate the development of antiviral drugs.
- **Genomics**
  - **Epitope analysis** – aims to support vaccine development.
  - **Host response analysis** – aims to identify additional drug targets in the host and to build models to attempt to predict which patients are likely to be at high risk.
  - **Virus Evolutionary Analysis** – aims to better understand the origin and structure of the virus genome





Virus spike structure as computed on Frontera, courtesy Rommie Amaro, UCSD

Courtesy Rick Stevens, U. of Chicago/ANL



AI-driven multi-[illegible] simulations of SARS-CoV-2

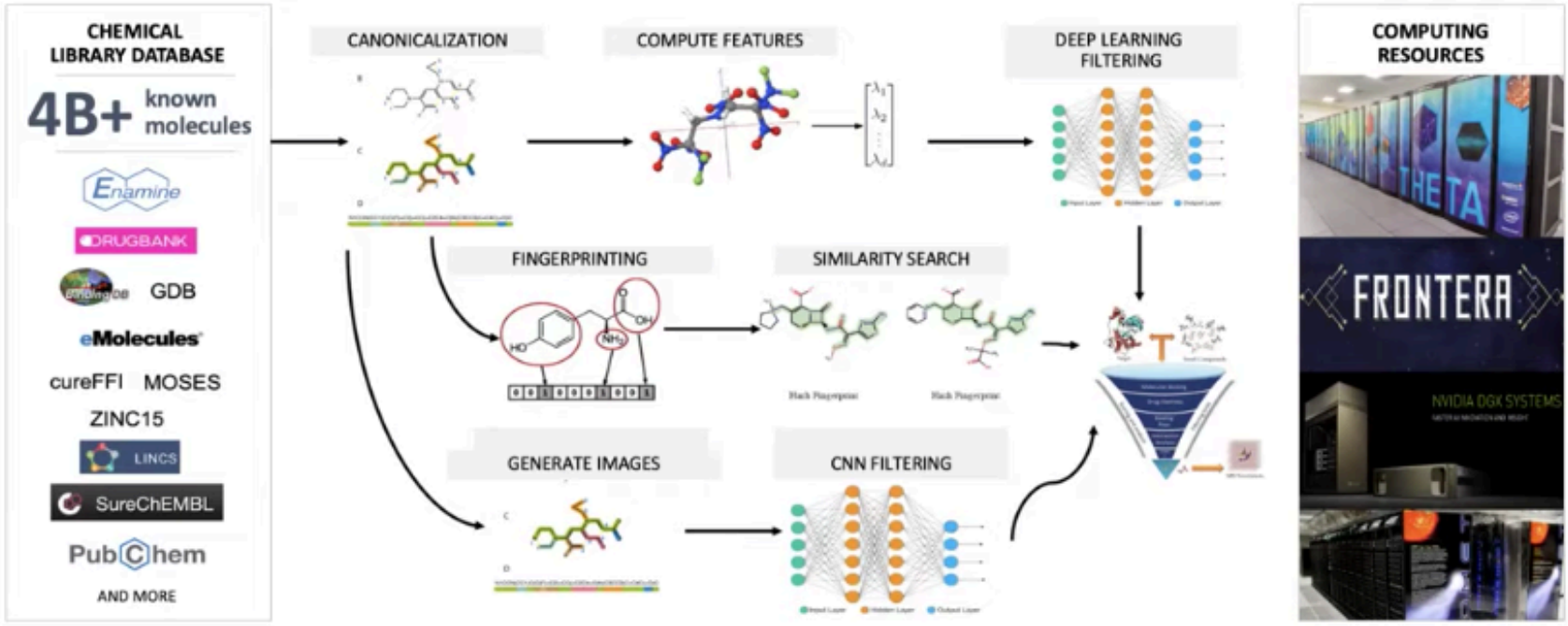
- All-atom viral envelope simulations are limited by timescales that are accessible
- Experimental data still challenging to integrate
- AI is used as a "glue" to drive adaptive sampling and improve accessible experimental observables
- Multi-resolution techniques implemented using FFEA:
  - intermediate representation from experimental data
  - AI builds automatic conversion across multiple scales

R. Amaro (UCSD), S. Harris (Leeds), C. Simmerling (Stony Brook), S. Jha (Rutgers/ Brookhaven)

CANDLE Team has been using CANDLE infrastructure to support large-scale docking and machine learning training and inference

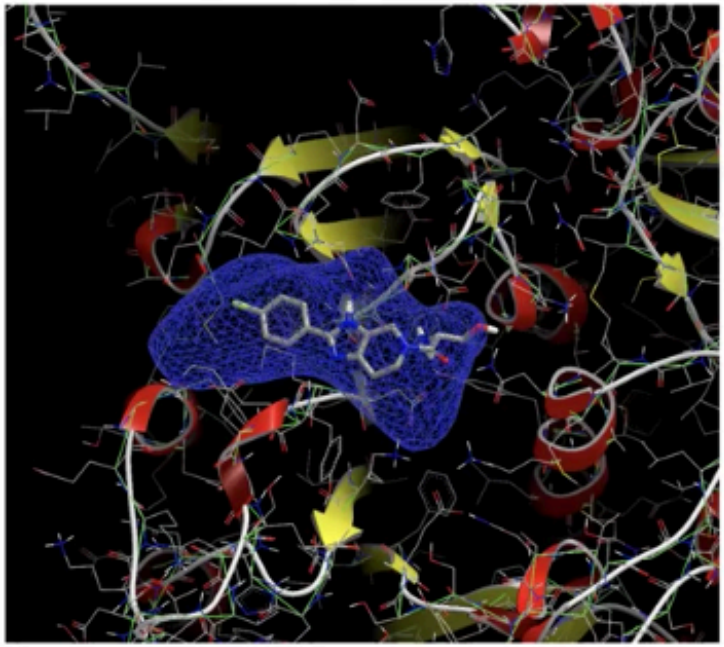
Courtesy Rick Stevens, U. of Chicago/ANL

AI and Supercomputers used to accelerate drug development

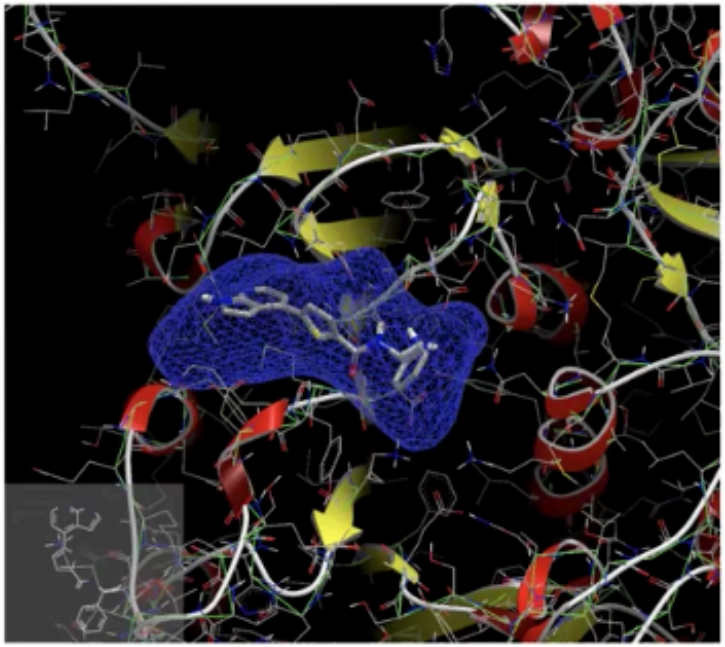


Example: NSP16 (6W61) 2’-O-Methyltransferase

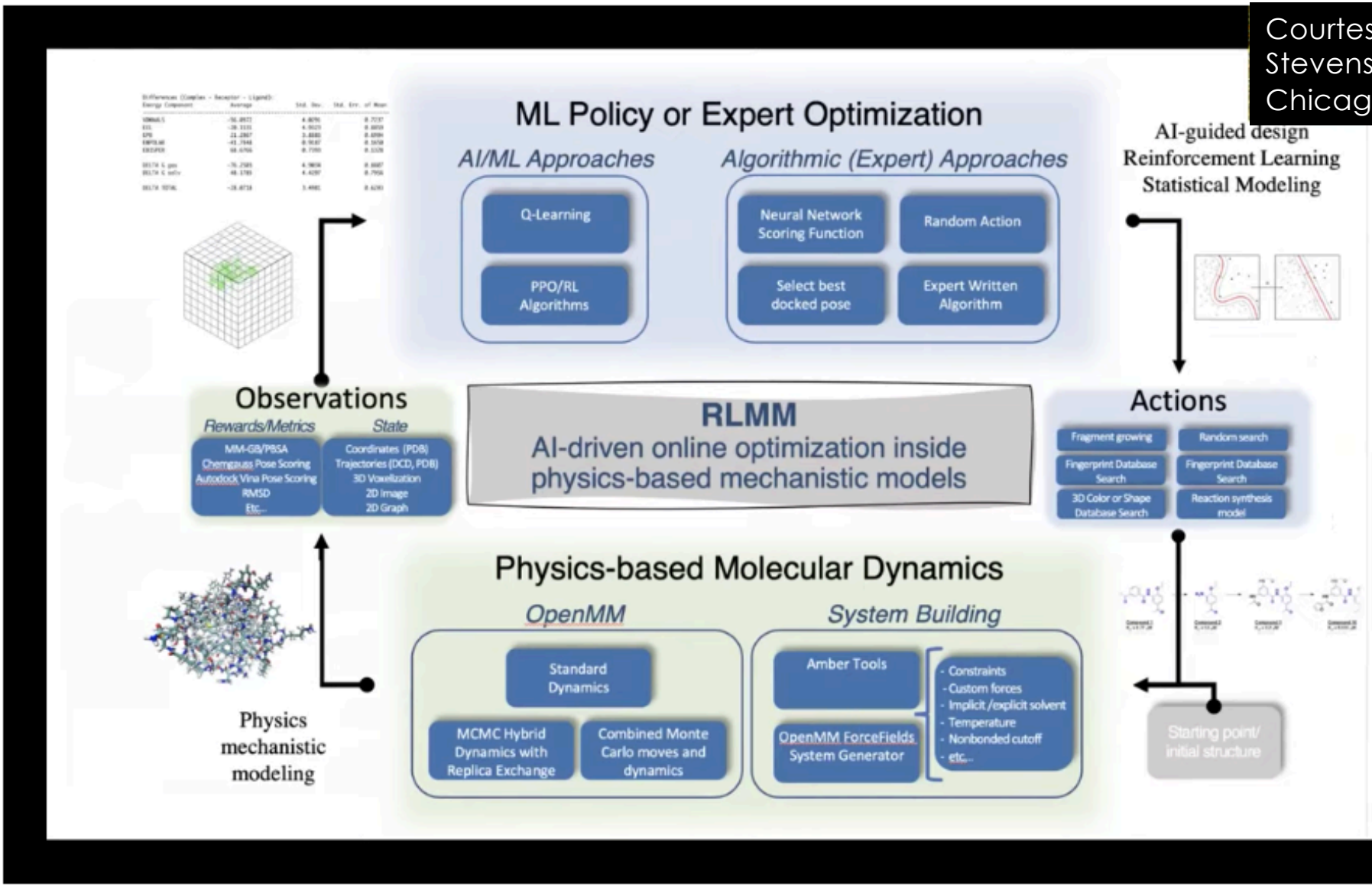
ZINC000215636639 Score -15.34
Top hit from > 6M orderable molecules



DB07812 Score -14.00
Known AKT2 Kinase Inhibitor (experimental drug)

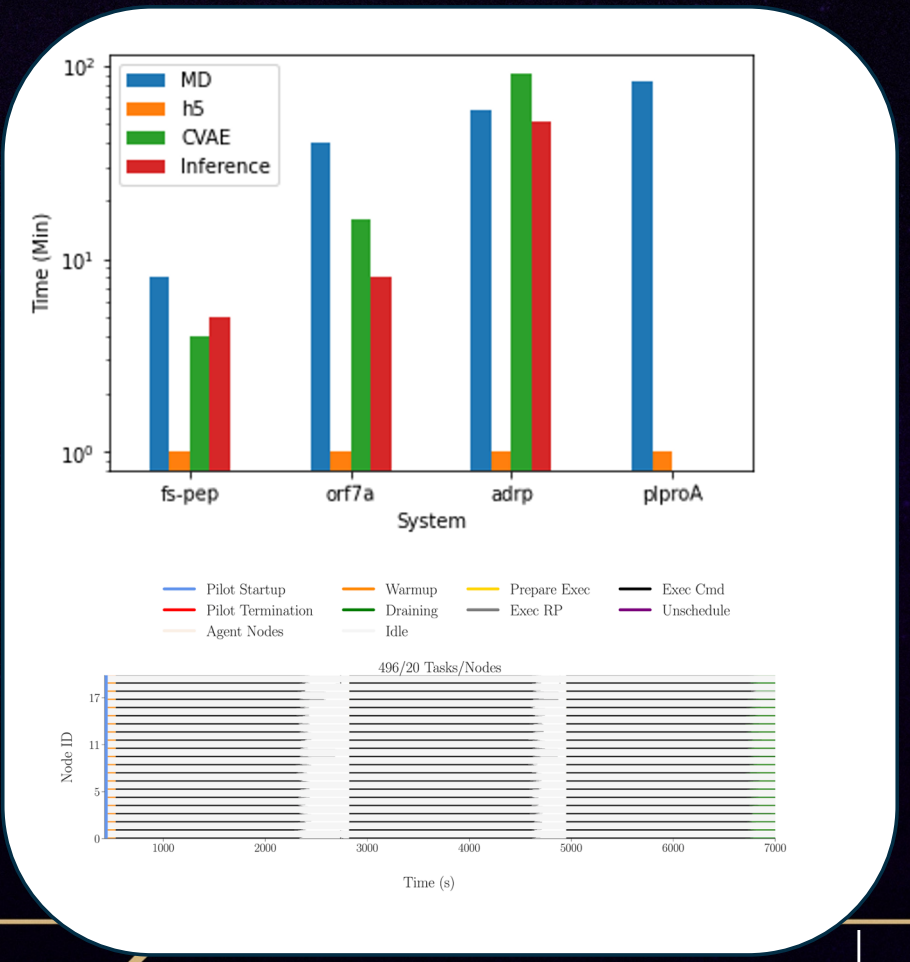


Courtesy Rick Stevens, U. of Chicago/ANL



AI-HPC INFRASTRUCTURE PERFORMANCE
(COURTESY SHANTENU JHA)

- **Stage-1**: ~20M SMILES/hour (Frontera)
  - Docking tasks have 2x fluctuations RCT load balances!
  - Scales to more 100,000 cores (i.e., 2000 nodes) on Frontera
- **Stage-2**: DeepDriveMD (Summit)
  - Summit: 20 nodes, 120 GPUs
  - Training time becomes increasingly challenging
  - 96% resource utilization although heterogeneous tasks are swapped
- **Stages-3** and **4**: ESMACS and TIES protocols use RCT individually but also are hybridized to efficiently use Summit nodes (6 GPUs + 42 CPU cores)
  - Efficiently executes >16K concurrent tasks on ≈ 2000 nodes (half of the entire Summit machine)



STILL TO COME

- For our Texas users:
  - Lonestar-5 will be replaced in early 2021 (Lonestar-6?)
  - Corral will also be refreshed/replace in early 2021
  - Longhorn (GPU) is available as part of our UT System support
- For all users:
  - Frontera Expansion this fall (extra COVID-19 capacity).
  - Chameleon hardware is being expanded/refreshed (GPU, CPU, SW defined networking)
  - Jetstream is getting a refresh in the spring.
  - Stampede-2 will continue until late 2022 – then something else will happen ☺.
  - Protected Data VM/Jupyter/Kubernetes Farm continues to grow.
- *And then. . .*

LEADERSHIP CLASS COMPUTING FACILITY

- In essence, our plan to transform the NSF and Open Science Computing Landscape from 2025-2035
- Construction set to begin 2023, Congress permitting.
- Datacenter expansion to 30MW, new and bigger systems, new approaches to storage and interactive, new buildings, staff expansion, more direct engagement in moving codes to new architectures
  - Relying on 50% software improvements to meet our targets.

LEADERSHIP-CLASS
COMPUTING FACILITY

THANKS!!

Mostly virtual, but still here!

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